Acetic acid, trifluoro-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 85.2 °C

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

Image not found
Acetic acid, trifluoro-
Measured: 73.0
Predicted: 85.2

Image not found
Flupropanate
Measured: 134
Predicted: 126

Image not found
Acetic acid, difluoro-
Measured: 133
Predicted: 132

Image not found
Pentafluoropropionic acid
Measured: 96.5
Predicted: 100

Image not found
Acetic acid, chlorodifluoro-
Measured: 122
Predicted: 128